

Chemical Data Visualization and Interactive Overlay's Module 104

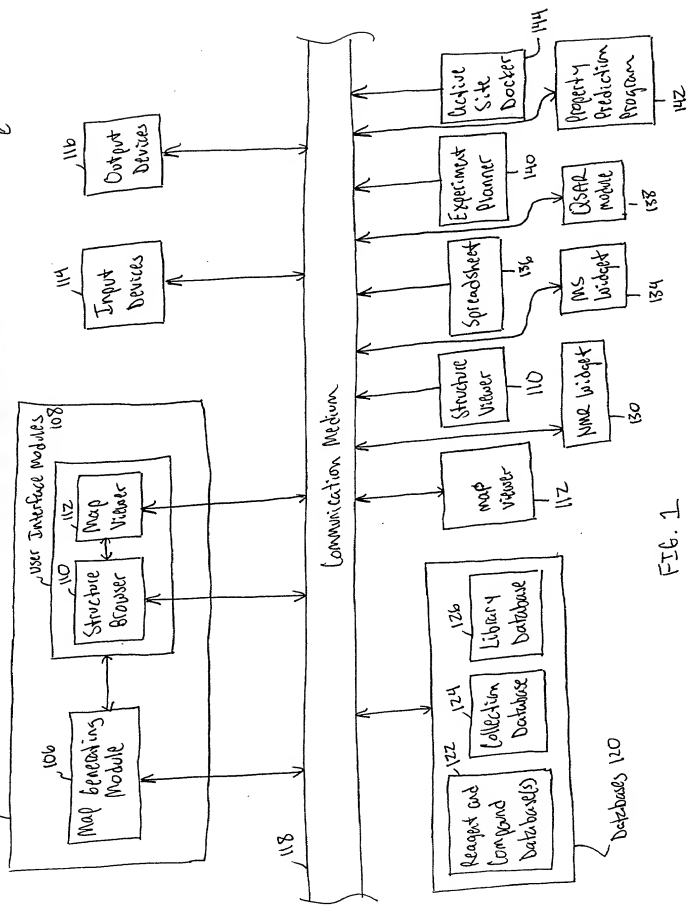


FIG. 1

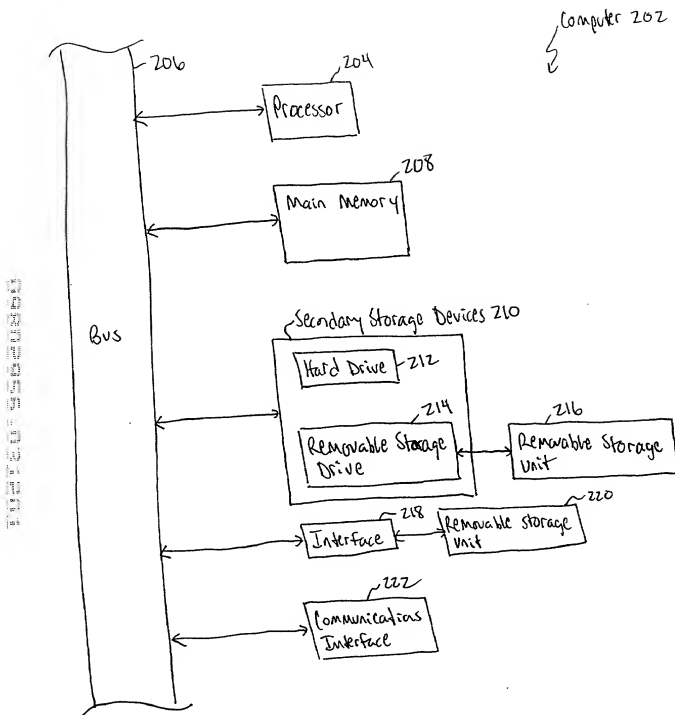


FIG. 2

302 ↘

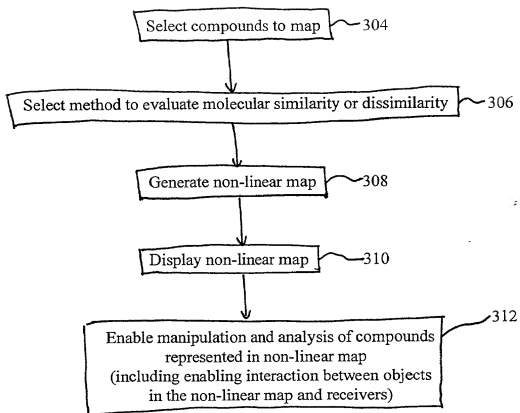


FIG. 3

402
↓

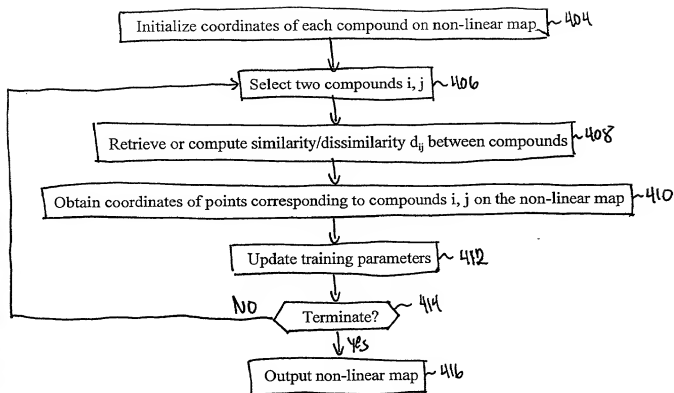
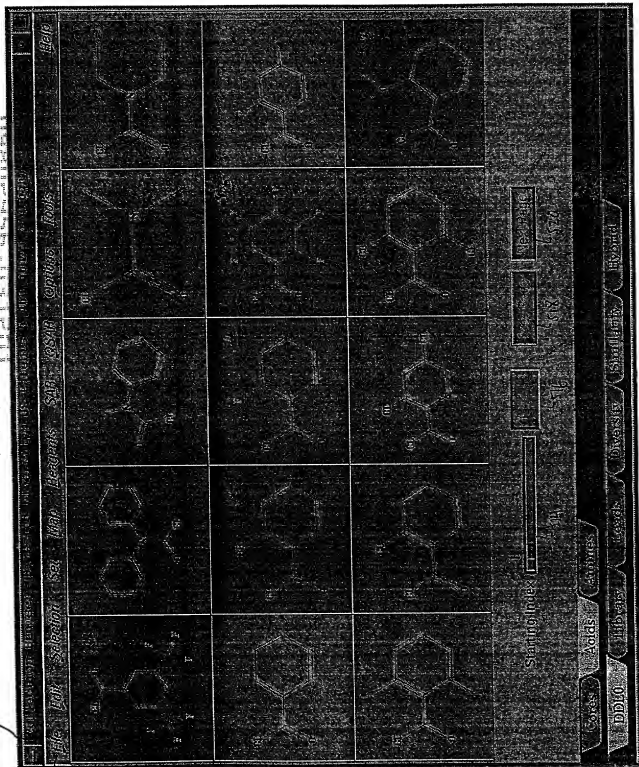


FIG. 4

FIG. 5



205

205

205

205
205
205

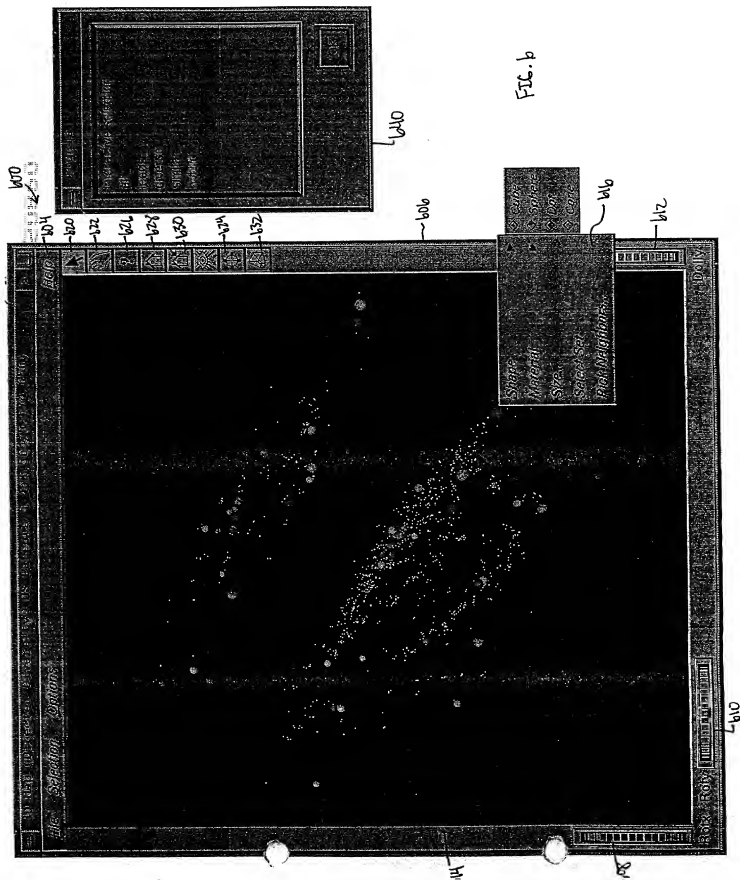
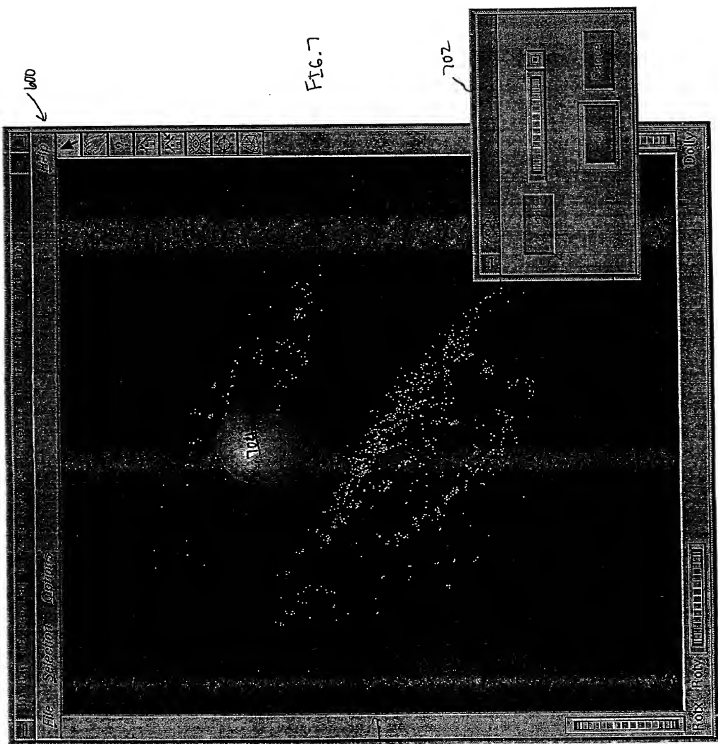


FIG. 6

FIG. 7



802

<div>Set Name</div> <div></div>		<div>Map Name</div> <div></div>		<div>Random Subse</div> <div><input checked="" type="checkbox"/></div>		<div>Mark</div> <div></div>		<div>OK</div>		<div>Cancel</div>	
<div>Set Name</div> <div></div>		<div>Map Name</div> <div></div>		<div>Random Subse</div> <div><input checked="" type="checkbox"/></div>		<div>Mark</div> <div></div>		<div>OK</div>		<div>Cancel</div>	

FIG. 8

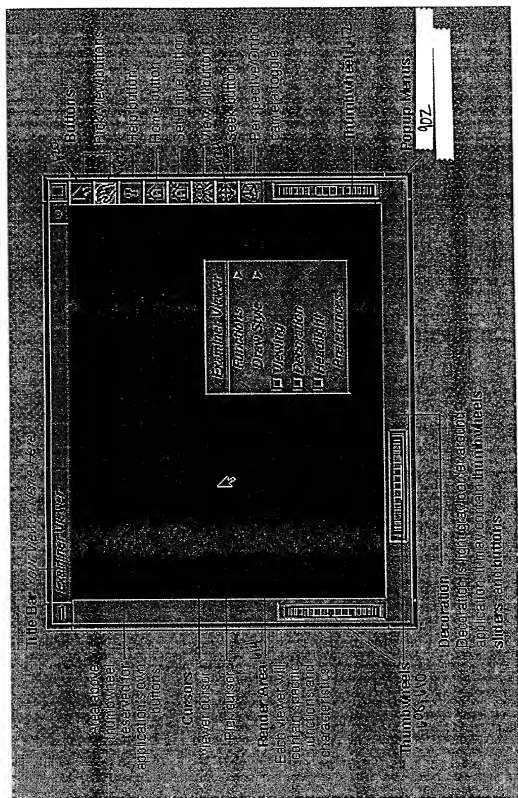


FIG. 9

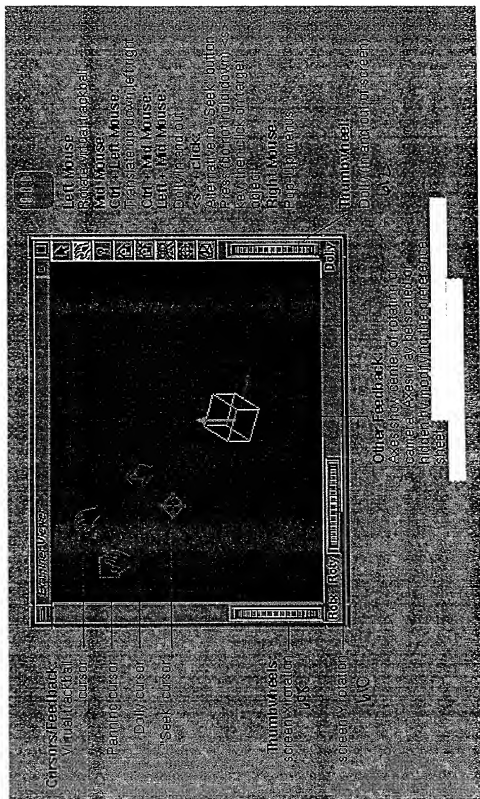


FIG. 10

1102

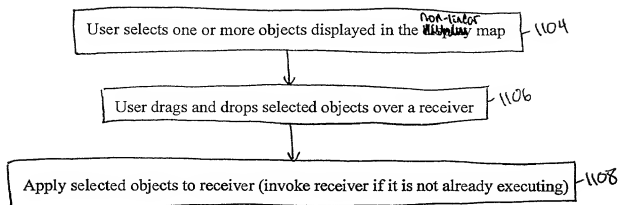


FIG. 11

1202

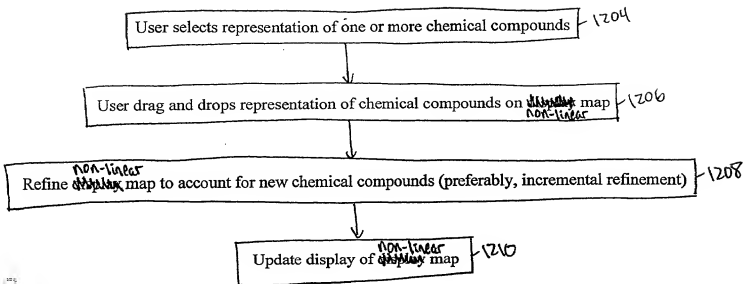
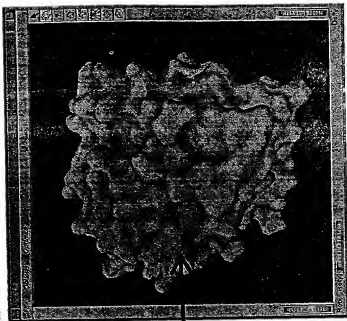
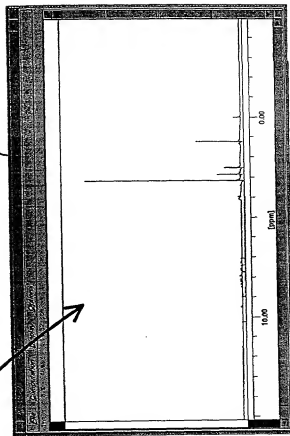


FIG. 12

Active Site Docker



NMR Viewer 130



3D Map Viewer

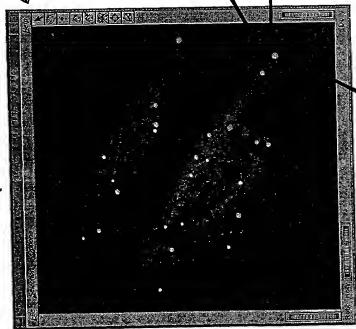
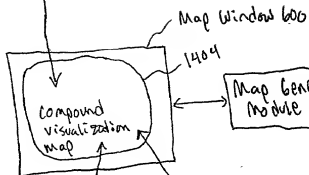
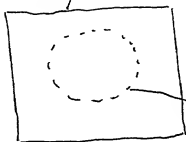


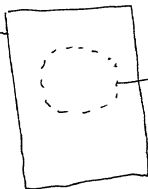
FIG. 13

Structure Browser 502
Window



Map Generating
Module 106

Compound
Database 122



MS viewer 1402

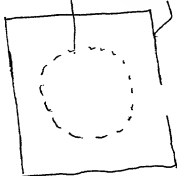


FIG. 14